

NIST SPECIAL PUBLICATION **260-133**

U.S. DEPARTMENT OF COMMERCE/Technology Administration  
National Institute of Standards and Technology

*Standard Reference Materials:*

**Acetylene  $^{12}\text{C}_2\text{H}_2$  Absorption Reference for  
1510–1540 nm Wavelength Calibration—  
SRM 2517**

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NO. 260-133

Sarah L. Gilbert and William C. Swann

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## Acetylene $^{12}\text{C}_2\text{H}_2$ Absorption Reference for 1510–1540 nm Wavelength Calibration— SRM 2517

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Standard Reference Materials:

**Acetylene  $^{12}\text{C}_2\text{H}_2$  Absorption Reference for 1510–1540 nm Wavelength Calibration – SRM 2517**

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**ABSTRACT**

Standard Reference Material (SRM) 2517 is an optical-fiber-coupled absorption cell containing acetylene ( $^{12}\text{C}_2\text{H}_2$ ) gas. It is intended for use in calibrating the wavelength scale of wavelength measuring instruments in the 1500 nm region. About 50 accurately measured absorption lines of the R and P branch of the  $\nu_1 + \nu_3$  rotational-vibrational band of  $^{12}\text{C}_2\text{H}_2$  are located between 1510–1540 nm. We have measured the pressure-induced shift of the lines and certify the SRM wavelengths with an expanded uncertainty (coverage factor  $k = 2$ ) of  $\pm 0.0006$  nm. This publication describes the SRM, the NIST measurement procedure, and the uncertainty determination for SRM certification.

**Keywords:** absorption; acetylene; molecular spectroscopy; optical fiber communication; Standard Reference Material; wavelength calibration; wavelength division multiplexing; wavelength reference; WDM

## 1. Introduction

Wavelength references are needed in the 1500 nm region to support future wavelength division multiplexed (WDM) optical fiber communication systems. In a WDM system, many wavelength channels are sent down the same fiber, thereby increasing the bandwidth of the system by the number of channels. If one channel's wavelength were to shift, crosstalk could occur between it and a neighboring channel. Wavelength references are needed to calibrate instruments that measure and set the wavelengths of the channels.

The NIST Optoelectronics Division has received numerous inquiries about wavelength calibration in the 1500 nm region. Most applications involve calibrating a commercial optical spectrum analyzer (OSA) which is based on the dispersion of light by a diffraction grating. An OSA typically has a resolution of 0.1 nm; the highest resolution currently available is 0.05 nm. Most users are interested in calibrating these instruments to an uncertainty between 0.1 and 0.01 nm. Many users are also interested in calibrating the wavelength scan linearity of their instruments. A calibration service did not seem practical for these instruments; they are large and fragile, and the optical elements can shift during shipment, causing a loss of wavelength calibration. The NIST solution is to produce Standard Reference Material (SRM) cells containing gases which have accurately measured absorption lines in this wavelength region. Fundamental molecular absorptions provide references which are very stable under changing environmental conditions such as temperature and pressure variations, or the presence of electric and magnetic fields. These SRMs can also be used to calibrate the wavelength readout of tunable lasers and check the accuracy of wavelength meters.

There are very few wavelength references available in the 1500 nm region. There is only one gas laser reference line: the 1523 nm helium-neon laser. The only atomic absorption lines in this region are between excited states and thus require initial excitation by a laser or electric discharge. Another possibility is frequency doubling 1500–1560 nm light to probe atomic transitions in the 750–780 nm region. This requires fairly complicated and expensive apparatus. Molecular transitions in the 1500 nm region are combination or overtone bands that can be probed directly.

We have chosen to use the absorption lines of acetylene (this SRM) and hydrogen cyanide (SRM 2519) for references in the 1500 nm region for the following reasons:

- (1) Molecular lines are simple to access, since this involves simply passing light through a cell containing the gas and observing the absorption spectrum.
- (2) These molecules have strong absorption bands in this region.
- (3) The combined spectra of the two gases cover the communications band, from 1510 to 1565 nm.
- (4) The spectra are uncomplicated; thus it is not difficult to identify the lines.
- (5) The wavelengths of the prominent lines have been measured with an uncertainty of less than 0.001 nm.
- (6) There are many reference lines with spacings ranging from 0.4 to 0.9 nm, providing for scan linearity calibration as well as single-point wavelength calibration.

- (7) A cell containing the gas can be easily pigtailed with optical fiber, so that it is compatible with the sources and measurement instruments used by the optical fiber communications industry.
- (8) The gas cell design allows for versatile calibration capability; it can be used with a variety of sources (LED, amplified spontaneous emission, white light, laser, etc.) to calibrate any wavelength measuring instrument in this region.

## 2. SRM 2517 description

This SRM is based on the fundamental absorptions of light by acetylene ( $^{12}\text{C}_2\text{H}_2$ ). The spectrum of this molecule in the 1500 nm region is shown in Fig. 1. The lines are the R and P branches of the  $\nu_1 + \nu_3$  rotational-vibrational band of  $^{12}\text{C}_2\text{H}_2$ . Figure 2 shows a schematic diagram of our apparatus for measuring the spectrum in Fig. 1. Light from an LED source (about 80 nm bandwidth) is coupled to an acetylene absorption cell using single-mode optical fiber. The light exiting the fiber is collimated by a lens, passes through the absorption cell, and is coupled into another section of single-mode fiber. This fiber is connected to a commercial optical spectrum analyzer. The resulting spectrum is the emission spectrum from the LED with narrow depressions due to the absorption of the light by the molecules. The spectrum in Fig. 1 has been normalized to the LED spectrum. We have also recorded the spectrum using a tunable laser as the light source. In this case the transmission through the cell was monitored by a detector as the laser's wavelength was tuned.

The vacuum wavelengths of the acetylene  $\nu_1 + \nu_3$  lines have been measured with an uncertainty of less than 0.0001 nm [1]. Table 1 lists the literature values for the wavelengths from 1513 to 1541 nm. We have compared these values with other experimental measurements in the literature [2,3] and find agreement within 0.0002 nm, which is within the expanded uncertainty of Refs. 2 and 3. Our measurements of six lines (below) also agree within our 0.0015 nm wavelength meter uncertainty.

## 3. SRM design

The SRM design is essentially that shown schematically in Fig. 2; an absorption cell is pigtailed with single-mode optical fiber. The input and output ports are FC/PC fiber bulkhead connectors on the outside of the instrument box. Users supply their own light source and detection; this enables flexibility since some users may want to calibrate optical spectrum analyzers using a broadband light source, and others may want to check the calibration of tunable lasers or wavelength meters using a narrowband source.

The absorption cell material is Pyrex glass; the windows are fused to the cell. The cell is first evacuated and leak-checked, and then filled with high purity gas (99.96%  $^{12}\text{C}_2\text{H}_2$ ). It is then tipped off using a torch, providing an all-glass seal. The cell is securely mounted in an aluminum holder. The fiber-coupled collimators are also mounted on this holder using commercially available aligners. FC/PC connectors on the other ends of the optical fibers connect to bulkhead connectors mounted on the instrument box which houses the cell holder.

We chose a pressure of 27 kPa (200 Torr) so that the lines would be pressure-broadened by less than 0.05 nm and thus provide a large signal, without significant loss of resolution, when used with instruments with this resolution. At this pressure, a slight shift of each line (pressure shift) is possible due to energy level shifts caused by the interaction of the molecules during elastic collisions [4]. An upper limit for the pressure shift of 200 kHz/Torr (1.5 kHz/Pa) has been reported for one acetylene line at low pressure [5]. We have measured the pressure shift of several lines, as described in section 4.1.

#### 4. Line center uncertainty

For this Standard Reference Material, the stability of the wavelength of each absorption line is a critical characteristic. The choice of fundamental molecular absorption lines makes the SRM insensitive to most changes in environmental conditions. The symmetric isotopic species of acetylene ( $^{12}\text{C}_2\text{H}_2$  and  $^{13}\text{C}_2\text{H}_2$ ) are particularly insensitive to changes because they have no permanent dipole moment. Thus, pressure broadening, pressure shift, and Stark shift are expected to be small. For the desired SRM certification uncertainty of about 0.001 nm, the only line shift mechanism which could potentially contribute at this level is the shift due to pressure (collisions between molecules). Other factors associated with line fitting could cause apparent shifts of lines. In section 4.1 we discuss our measurement of the pressure shift.

##### 4.1 Pressure shift measurement

A schematic diagram of our pressure shift measurement apparatus is shown in Fig. 3. Light from a tunable diode laser is sent through two absorption cells simultaneously, and the transmission through each cell is monitored by a detector. One cell contains acetylene gas at low pressure ( $8.0 \pm 0.8$  kPa; about 60 Torr) and the other contains a relatively high pressure of  $54 \pm 5$  kPa (about 400 Torr). The pressure uncertainty quoted is the expanded uncertainty using a coverage factor  $k = 2$ . A wavelength meter with an uncertainty of 1 part in  $10^6$  (0.0015 nm) monitors the wavelength of the laser. A computer scans the wavelength of the laser in approximately 0.001 nm steps and records the two detectors and wavelength meter readings.

Figure 4 shows the spectrum obtained of line P5. The pressure broadening in the high-pressure cell is obvious. We are interested in the relative shift between the line centers in the low-pressure and high-pressure cells. Six lines were recorded using this technique. The measured quantity, the transmitted power  $I_t$ , is related to the absorption coefficient  $\alpha$  and the absorption path length  $L$  by

$$I_t = I_o \exp(-\alpha L), \quad (1)$$

where  $I_o$  is the incident power. We first normalized the data to  $I_o$  and then took the natural logarithm to obtain  $\alpha L$ . The low pressure lines were fitted to a Voigt profile [6] using the least-squares method of a commercial fitting program. Due to the dominance of pressure broadening in the high pressure cell, these lines were fitted to a Lorentzian profile. Several factors complicated the fitting procedure: overlap with nearby lines, background slopes, interference fringes on the cell transmission spectra, and uncertainty in the wavelength of each point. Our approach to minimizing and measuring the effects of these contributions is discussed below.



#### 4.1.1 Overlap with nearby lines

Wings of nearby lines can skew the shape of the line being measured and shift its apparent center. There are a number of weak lines throughout the spectrum which are due to hot bands (transitions that are not out of the ground vibrational state) [7]. To account for the weak nearby lines, we did a multiple-line fit to the low pressure cell spectrum (Fig. 5a – spectrum inverted) and then used the line locations and strengths obtained in this fit as input to a multiple-line fit of the high pressure cell spectrum (Fig. 5b). A multiple-line fit is simply a fit to a sum of lines instead of a single line. For the spectra shown in Figs. 5a and 5b, the multiple-line fit consisted of the main line near 1528.6 nm and three weak lines at longer wavelengths. After modeling the weak lines, we subtracted them from the data to obtain a spectrum that contained only the main line. This modified spectrum could then be fit more accurately with the appropriate error bars. We estimated the uncertainty in this process by visibly changing the center wavelength parameter of the nearest line and refitting the data with this parameter fixed. This resulted in a negligible shift of the main line for the low pressure cell data and a maximum shift of  $\pm 0.0002$  nm for the high pressure cell data. Assuming a rectangular distribution with upper and lower limits of  $\pm 0.0002$  nm about the mean value, this corresponds to a standard uncertainty (estimated standard deviation)  $u$  of  $0.0001$  nm ( $=0.0002/\sqrt{3}$ ).

#### 4.1.2 Background slope

A background slope on the spectrum can shift the apparent center of a line, particularly for the wide lines of the high pressure cell. We have identified two sources of background slope: (1) wavelength dependence of the fiber couplers and other optical components, and (2) change in the laser power. Since the magnitudes of the background slopes were small, we chose to fit the data without removing the slopes. Slight residual slopes in the data could be seen in the fit residual plots. By fitting the data again with the slope removed, we calculate that the maximum shift due to any residual slope is negligible for the low pressure cell data and  $\pm 0.0002$  nm for the high pressure cell data. Assuming a rectangular distribution with upper and lower limits of  $\pm 0.0002$  nm about the mean value, this corresponds to a standard uncertainty  $u$  of  $0.0001$  nm.

#### 4.1.3 Interference fringes

Interference fringes due to reflections of the laser light can be a problem. We spent considerable time reducing these effects. The windows of the cells were mounted at a  $10^\circ$  angle with respect to the laser beam path. We selected low back-reflection fiber-pigtailed lenses and terminated the fibers (at the detectors) with angled fiber connectors. These measures reduced the interference fringe amplitude considerably. The amplitudes of the remaining fringes were less than 0.2%. We modeled the effect of the fringes by simulating lines with and without the modulation and fitting the simulated data to obtain the line centers. Using the worst-case scenario for the phase of the modulation relative to the line center, we calculate a maximum apparent line shift of  $\pm 0.00001$  nm for the low pressure cell data and  $\pm 0.0004$  nm for the high pressure cell data. Assuming a rectangular distribution with upper and lower limits of  $\pm 0.0004$  nm about the mean value, this corresponds to a standard uncertainty  $u$  of  $0.0002$  nm for the high pressure cell data.

#### 4.1.4 Wavelength uncertainty

Since the transmissions through the low and high pressure cells were measured simultaneously, the accuracy of the wavelength meter was adequate for this measurement. However, its limited resolution (0.001 nm) did add noise to the data. This, in turn, complicated the fitting since there was noise in both  $y$  (transmitted intensity) and  $x$  (wavelength), and our fitting program could accommodate uncertainty in  $y$  only. Since the transmission is a complicated function of wavelength, uncertainty of the wavelength has the largest effect where the transmission slope is the greatest. Our approach to estimating the uncertainty in each data point was to first fit the data with a Lorentzian lineshape [8]. We then took the derivative of this function with respect to wavelength and from that derived a virtual uncertainty in the transmission  $T$  due to this wavelength dependence:

$$\delta T_{\lambda} \approx \left| \frac{\partial T}{\partial \lambda} \right| \delta \lambda. \quad (2)$$

We then combined this uncertainty with the uncertainty due to intensity variation (measured experimentally) for the overall estimate of uncertainty for each transmission measurement point.

### 5. Uncertainty determination

We measured the pressure shifts for six different lines, choosing lines at a variety of locations in the spectrum. This ensured that our data would be sensitive to any variations in the pressure shift, if the shift varied with line number. We obtained reduced residual-sum-of-squares ( $\chi^2$ ) values ranging from 0.9 to 2.6 for the fitting of six lines. From the fit residual plots, we could discern the slight slopes and sinusoidal modulation described above; fitting and removing these slopes and modulations reduced the  $\chi^2$  values to 0.8 - 1.1. As discussed above, we used the line center values obtained from fitting without the slopes and modulations removed, since we do not think it was justified to arbitrarily remove these effects. Instead, we used the residual plots to estimate the uncertainty in the line centers. The magnitudes of the slopes and modulations in the residual plots were consistent with background data taken with the cells removed from the measurement apparatus.

The uncertainty budget for the relative line center determinations is given in Table 2 and the uncertainty source type [9] (A or B) is indicated. The largest source of uncertainty is the apparent shift due to interference fringes. Table 3 lists the shifts measured for six lines. Since it is possible that the pressure shifts for the different lines are slightly different, we use the average of the pressure shifts measured, and combine the individual shift standard uncertainty  $u_c(\Delta)$  with the standard deviation of the six line shifts  $u(\text{six})$  using the a root-sum-of-squares (RSS) method to obtain the overall line shift standard uncertainty of 0.0005 nm.

Unless otherwise stated, the uncertainties given below are all expanded uncertainties using a coverage factor  $k = 2$ . Our result is a pressure shift of  $0.0015 \pm 0.0010$  nm for a pressure difference of  $46 \pm 5$  kPa ( $345 \pm 40$  Torr); yielding  $(+ 3.2 \pm 2.2) \times 10^{-5}$  nm/kPa [ $(+ 4.3 \pm 2.9) \times 10^{-6}$  nm/Torr], or  $- 4.1 \pm 2.8$  MHz/kPa ( $- 0.55 \pm 0.37$  MHz/Torr).

For the  $27 \pm 7$  kPa ( $200 \pm 50$  Torr) pressure used in the SRM units, the pressure shift is  $+0.0009 \pm 0.0006$  nm. Table 4 lists the certified wavelengths for the SRM units. We obtain these wavelengths by adding the pressure shift to the literature values given in Table 1.

## 6. SRM 2517 certificate

The certificate for SRM 2517 is presented in Appendix A. It includes the certified wavelength values for the  $\nu_1 + \nu_3$  band of  $^{12}\text{C}_2\text{H}_2$  ranging from R25 to P25 (1513-1541 nm), a scan of the band, and instructions for storage, handling, and use of the SRM.

## 7. Acknowledgment

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**Table 1. Vacuum Wavelengths of Acetylene  $^{12}\text{C}_2\text{H}_2$  Lines**

The wavelengths were calculated using the experimentally determined molecular constants from Ref. 1, and were compared with less accurate measurements (Refs. 2 and 3). The wavelength uncertainty estimate given in Ref. 1 is  $1 \times 10^{-6}$  nm (one standard uncertainty).

R Branch	wavelength (nm)	P Branch	wavelength (nm)
25	1513.1999	1	1525.7598
24	1513.5830	2	1526.3138
23	1513.9725	3	1526.8742
22	1514.3682	4	1527.4410
21	1514.7702	5	1528.0142
20	1515.1785	6	1528.5938
19	1515.5930	7	1529.1798
18	1516.0139	8	1529.7722
17	1516.4411	9	1530.3710
16	1516.8746	10	1530.9762
15	1517.3144	11	1531.5878
14	1517.7605	12	1532.2059
13	1518.2129	13	1532.8303
12	1518.6716	14	1533.4613
11	1519.1367	15	1534.0986
10	1519.6081	16	1534.7424
9	1520.0858	17	1535.3927
8	1520.5699	18	1536.0493
7	1521.0603	19	1536.7125
6	1521.5570	20	1537.3821
5	1522.0601	21	1538.0582
4	1522.5696	22	1538.7407
3	1523.0854	23	1539.4298
2	1523.6075	24	1540.1253
1	1524.1360	25	1540.8273



**Table 2. Uncertainty Budget**

Uncertainty budget for determination of relative line centers for the low pressure and high pressure cells. The combined standard uncertainties are root-sum-of-squares (RSS) of the standard uncertainties due to the sources listed. The absolute accuracy of the wavelength meter is not included since we are concerned only with the relative line centers.

Source of uncertainty	Uncertainty type [9]	Standard uncertainty (nm) 8 kPa ( <i>low</i> ) cell	Standard uncertainty (nm) 54 kPa ( <i>high</i> ) cell
Nearby line contribution	B	< 0.00001	0.0001
Background slope	B	< 0.00001	0.0001
Interference fringes	B	< 0.00001	0.0002
Fit statistical uncertainty	A	0.0001	0.0001
Combined standard uncertainty		$u_c(\text{low}) = 0.0001$	$u_c(\text{high}) = 0.0003$

**Table 3. Pressure Shift Measurement**

Measured center wavelengths and shifts for six lines of  $^{12}\text{C}_2\text{H}_2$ . The individual line shift standard uncertainty  $u_c(\Delta)$  is the RSS combined uncertainty of  $u_c(\text{low})$  and  $u_c(\text{high})$  from Table 2. The lines in the high pressure cell are shifted by an average of + 0.0015 nm relative to the lines in the low pressure cell.

Line	Measured center $\lambda$ (nm) 8 kPa ( <i>low</i> ) cell	Measured center $\lambda$ (nm) 54 kPa ( <i>high</i> ) cell	Shift (nm) [ $\Delta = \text{high} - \text{low}$ ]	Shift standard uncertainty $u_c(\Delta)$ (nm)
R18	1516.0130	1516.0150	+ 0.0020	0.0003
P3	1526.8738	1526.8749	+ 0.0011	0.0003
P5	1528.0136	1528.0154	+ 0.0018	0.0003
P6	1528.5934	1528.5950	+ 0.0016	0.0003
P14	1533.4604	1533.4619	+ 0.0015	0.0003
P25	1540.8270	1540.8278	+ 0.0008	0.0003
Average shift			+ 0.0015	

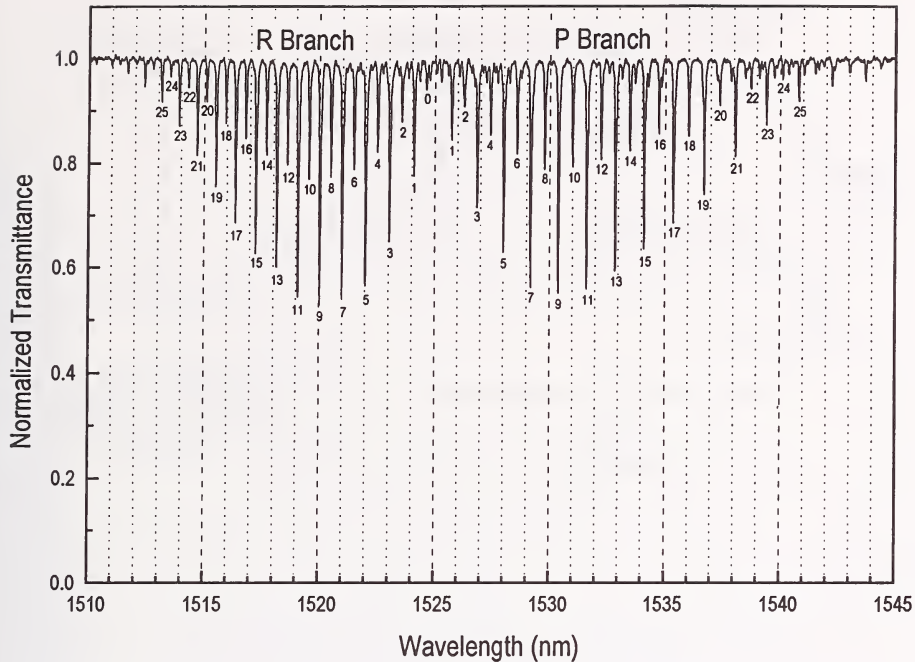
Standard deviation of six lines,  $u(\text{six})$  0.0004 nm

Shift overall combined standard  
uncertainty  $[(u(\text{six}))^2 + (u_c(\Delta))^2]^{1/2}$  0.0005 nm

**Table 4 Certified Wavelengths for SRM 2517**

Literature values from Ref. 1 adjusted for the pressure shift due to the 27 kPa (200 Torr) cell pressure. These vacuum wavelengths of the  $\nu_1 + \nu_3$  band  $^{12}\text{C}_2\text{H}_2$  are certified with an expanded uncertainty of  $\pm 0.0006$  nm (coverage factor  $k = 2$ ).

R Branch	wavelength (nm)	P Branch	wavelength (nm)
25	1513.2007	1	1525.7607
24	1513.5839	2	1526.3147
23	1513.9733	3	1526.8751
22	1514.3690	4	1527.4419
21	1514.7710	5	1528.0151
20	1515.1793	6	1528.5946
19	1515.5939	7	1529.1806
18	1516.0148	8	1529.7730
17	1516.4419	9	1530.3718
16	1516.8754	10	1530.9770
15	1517.3152	11	1531.5886
14	1517.7613	12	1532.2067
13	1518.2138	13	1532.8312
12	1518.6725	14	1533.4621
11	1519.1376	15	1534.0995
10	1519.6090	16	1534.7433
9	1520.0867	17	1535.3935
8	1520.5707	18	1536.0502
7	1521.0611	19	1536.7134
6	1521.5579	20	1537.3830
5	1522.0610	21	1538.0590
4	1522.5704	22	1538.7416
3	1523.0862	23	1539.4306
2	1523.6084	24	1540.1261
1	1524.1369	25	1540.8281



**Figure 1.** Acetylene ( $^{12}\text{C}_2\text{H}_2$ ) spectrum taken by passing LED light through an absorption cell and recording the spectrum of the transmitted light using an optical spectrum analyzer with 0.05 nm resolution. This spectrum has been divided by the LED spectrum.

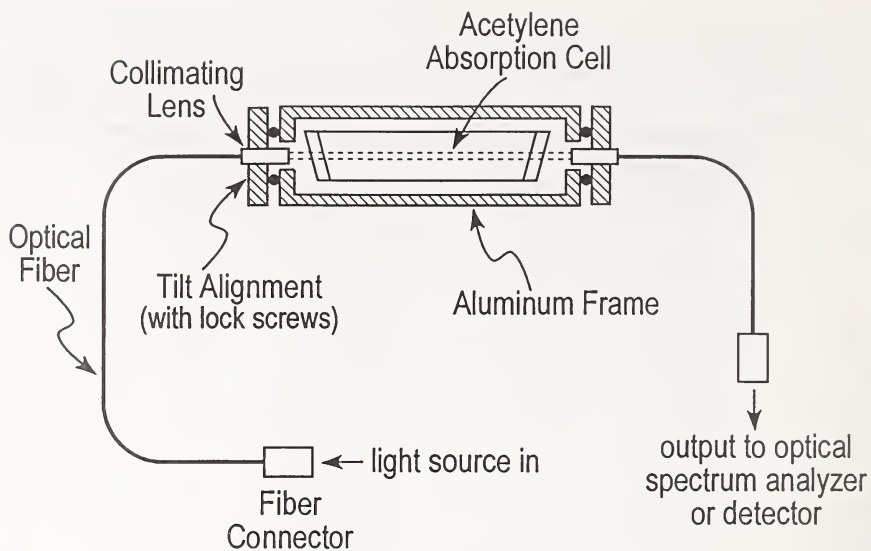
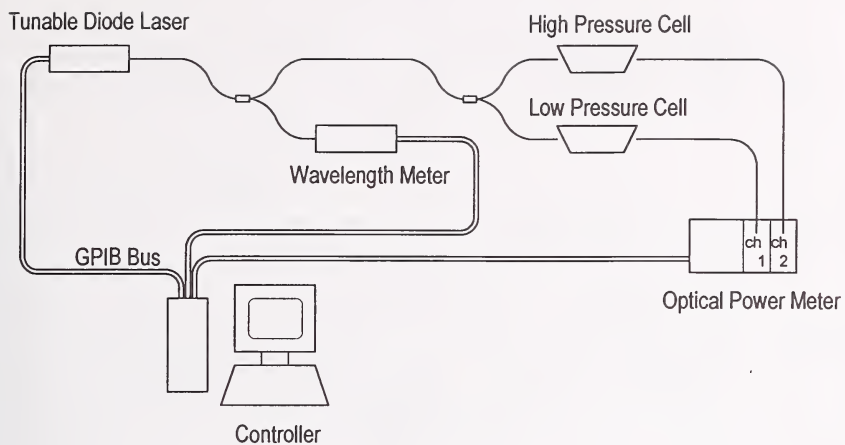


Figure 2. Schematic of fiber-pigtailed cell holder.





**Figure 3.** Schematic of the pressure-shift measurement apparatus.

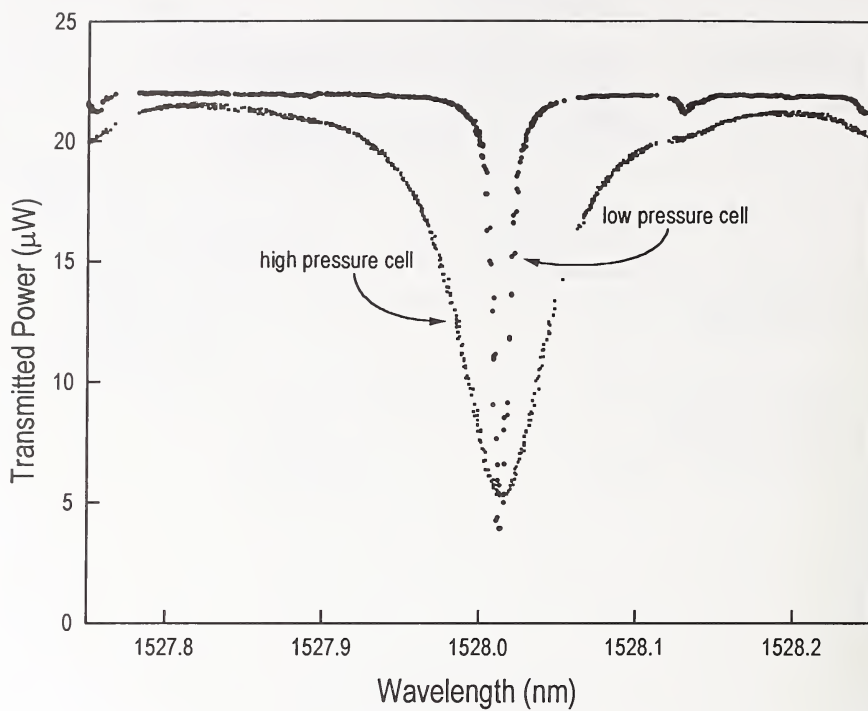


Figure 4. Scan over line P5 showing transmission through low pressure and high pressure cells.

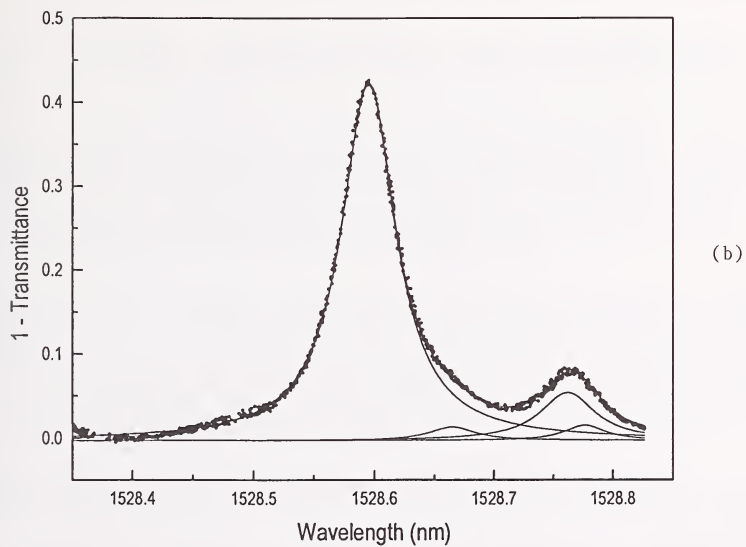
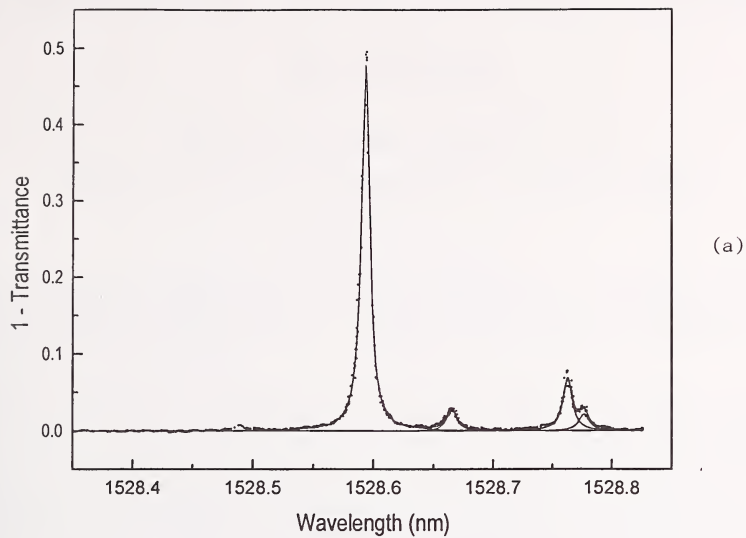


Figure 5. (a) Multiple line fit of line P6, low pressure cell. Of all the lines measured, P6 had the most significant contribution from nearby lines. (b) Multiple line fit of line P6, high pressure cell.





# National Institute of Standards & Technology

## Certificate

### Standard Reference Material® 2517

#### Wavelength Reference Absorption Cell – Acetylene ( $^{12}\text{C}_2\text{H}_2$ )

Serial No.:

This Standard Reference Material (SRM) is intended for use in calibrating the wavelength scale of wavelength measuring equipment in the spectral region from 1513 nm to 1541 nm. SRM 2517 is an optical-fiber-coupled absorption cell containing acetylene ( $^{12}\text{C}_2\text{H}_2$ ) gas. Acetylene has more than 50 accurately measured absorption lines in the 1500 nm wavelength region.

**Certified Wavelength Values:** The vacuum wavelengths of absorption lines in the R and P branch of the  $\nu_1 + \nu_3$  rotational-vibrational band of  $^{12}\text{C}_2\text{H}_2$  have been measured previously to high accuracy by several independent research groups [1,2]. These literature values for the vacuum wavelengths were adjusted for the pressure shift due to the collisions between acetylene molecules at the 27 kPa (200 Torr) pressure within the SRM cell to obtain the certified wavelength values for this SRM. Details of the measurement procedure and data analysis for the determination of the pressure shift can be found in reference [3]. A spectrum of the absorption band is shown in Figure 1 and certified wavelength values are given in Table 1. Figure 2 shows a higher resolution scan near line P9. The wavelengths of the lines listed in Table 1 are certified with an expanded uncertainty of  $\pm 0.0006$  nm (coverage factor  $k = 2$ ).

**Expiration of Certification:** The certification of this SRM is indefinite within the measurement uncertainties specified, provided the SRM is handled, stored, and used in accordance with the instructions given in this certificate.

**Measurement Conditions and Procedure:** The long term stability of acetylene and the use of fundamental molecular absorption lines render the SRM insensitive to changes in environmental conditions. The purpose of the certification procedure is to verify that the unit contains the correct pressure of  $^{12}\text{C}_2\text{H}_2$  gas and has no significant contaminants that produce additional absorption lines. Measurements were made using a 0.05 nm resolution optical spectrum analyzer. Spectra similar to those shown in Figures 1 and 2 were taken of each SRM unit and compared with measurements of reference absorption cells maintained at NIST.

**Storage and Handling:** The protective caps provided for the FC/PC fiber connectors should be replaced when the SRM is not in use. This SRM is intended to be used in a laboratory environment near ambient room temperature ( $22\text{ }^\circ\text{C} \pm 5\text{ }^\circ\text{C}$ ). Optical alignment is critical; the user should avoid exposing the unit to large temperature variations, temperature cycling, or mechanical shock, as these may cause the optical alignment to degrade. Optical misalignment affects the throughput of the SRM but will not shift the centers of the absorption lines. A more serious, but less likely problem is cell breakage or leakage. The unit should be replaced if the linewidths or depths differ significantly from those shown in Figures 1 and 2 (when measured using comparable resolution).

Development of the SRM and supporting measurements were performed by S.L. Gilbert and W.C. Swann of the NIST Optoelectronics Division.

Gaithersburg, MD 20899  
Certificate Issue Date: 20 October 1997

Thomas E. Gills, Chief  
Standard Reference Materials Program



Statistical consultation was provided by C.M. Wang of the NIST Statistical Engineering Division.

The support aspects involved in the preparation, certification, and issuance of this SRM were coordinated through the Standard Reference Materials Program by R.J. Gettings.

Table 1. Certified Wavelengths for SRM 2517

Literature values from Reference [1] adjusted for the pressure shift due to the 27 kPa (200 Torr) cell pressure. These vacuum wavelengths of the  $\nu_1 + \nu_3$  band of  $^{12}\text{C}_2\text{H}_2$  are certified with an expanded uncertainty of  $\pm 0.0006$  nm (coverage factor  $k = 2$ ).

R Branch	nm	P Branch	nm
25	1513.2007	1	1525.7607
24	1513.5839	2	1526.3147
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12	1518.6725	14	1533.4621
11	1519.1376	15	1534.0995
10	1519.6090	16	1534.7433
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6	1521.5579	20	1537.3830
5	1522.0610	21	1538.0590
4	1522.5704	22	1538.7416
3	1523.0862	23	1539.4306
2	1523.6084	24	1540.1261
1	1524.1369	25	1540.8281

**General Considerations:** The SRM can be used to calibrate a wavelength measuring instrument in the 1510 nm to 1540 nm region. The wavelength calibration is vacuum wavelength; if the user requires the wavelength in air, the appropriate correction for the index of refraction of air must be applied (see Reference [4]). Depending on what type of instrument is being calibrated, a broadband source or a tunable narrowband source may be used.

**Use With a Broadband Source:** A broadband source in the 1500 nm region (such as a light emitting diode, white light, or amplified spontaneous emission source) is useful when calibrating a low resolution instrument such as a diffraction grating based optical spectrum analyzer or monochromator. A schematic for this type of calibration is shown in Figure 3(a). Light from the broadband source is coupled into the SRM and the output (transmission through the SRM) is connected to the instrument that is being calibrated. The absorption lines of acetylene appear as dips in the spectrum of the light source (see Figure 1).

**Use With a Narrowband Source:** The SRM can be used to calibrate the wavelength scale of a tunable narrowband source in this region (such as a diode laser or fiber laser). Alternatively, a tunable source and the SRM can be used to check the calibration of a wavelength meter, as shown in Figure 3(b). The laser is tuned over one or more of the acetylene absorption lines. The transmission through the SRM is monitored by a detector; the transmitted power passes through a minimum at the center of an absorption line.

**Suggested Procedure for Low-Accuracy Requirements; Calibration Uncertainty  $\geq 0.1$  nm:** Connect the light source (either broadband or narrowband, as discussed above) to one of the fiber connectors on the SRM unit using a single-mode optical fiber terminated with a clean FC/PC connector. After identifying the absorption lines by comparing to the spectrum in Figure 1, find the center or the minimum point of a line listed in Table 1. If the instrument has variable resolution, it is best to use a resolution of  $\leq 0.2$  nm. For this level of accuracy, the procedure used to find the line center can be quite simple: setting a cursor to the line center or minimum by eye is sufficient. If using a tunable source, simply tune it to the transmission minimum of the line, using tuning steps of  $\leq 0.01$  nm. Calibrate the instrument to the wavelength of this line (from Table 1) using the calibration procedure specified by the instrument manufacturer. The instrument's linearity can be checked by repeating the procedure for a different absorption line and comparing it to the value listed in Table 1.

**Suggested Procedure for Moderate-Accuracy Requirements; Calibration Uncertainty in the Approximate Range of 0.01 nm to 0.1 nm:** Connect the light source (either broadband or narrowband, as discussed above) to one of the fiber connectors on the SRM unit using a single-mode optical fiber terminated with a clean FC/PC connector. If the source power varies significantly with wavelength, divide the SRM transmission spectrum by the source spectrum to obtain a normalized trace. After identifying the absorption lines by comparing to the spectrum in Figure 1, make a high resolution scan of a line listed in Table 1. If the instrument has variable resolution, it is best to use a resolution of  $\leq 0.1$  nm with a data point density of at least one point every 0.005 nm. Find the wavelength readings on both sides of the line where the absorption is 50 % of the maximum; the line center is half-way between these two wavelength readings. Repeat this procedure five times and take the average of the five measurements for the line center. Calibrate the instrument to the center wavelength of this line (from Table 1) using the calibration procedure specified by the instrument manufacturer. The instrument's linearity can be checked by repeating the procedure for a different absorption line and comparing it to the value listed in Table 1.

**Suggested Procedure for High-Accuracy Requirements; Calibration Uncertainty  $\leq 0.01$  nm:** *[Note: due to the presence of weak nearby lines, background slope, and interference fringes, this SRM is not recommended for a calibration with an uncertainty of less than 0.001 nm.]* Connect the light source (either broadband or narrowband, as discussed above) to one of the fiber connectors on the SRM unit using a single-mode optical fiber terminated with a clean FC/PC connector. Divide the SRM transmission spectrum by the source spectrum to obtain a normalized trace. After identifying the absorption lines by comparing to the spectrum in Figure 1, make a high resolution scan of a line listed in Table 1. If the instrument has variable resolution, it is best to use a resolution of  $\leq 0.1$  nm with a data point density of at least one point every 0.001 nm. Using a fitting technique such as the least squares technique, fit the absorption data to the appropriate lineshape (Lorentzian if the line shape is dominated by the molecular absorption profile, Lorentzian convoluted with the instrument's filter characteristics if the instrument contributes significantly to the profile). Details of line fitting procedure and potential errors sources can be found in Reference [3]. Calibrate the instrument to the center wavelength of this line (from Table 1) using the calibration procedure specified by the instrument manufacturer. The instrument's linearity can be checked by repeating the procedure for a different absorption line and comparing it to the value listed in Table 1.

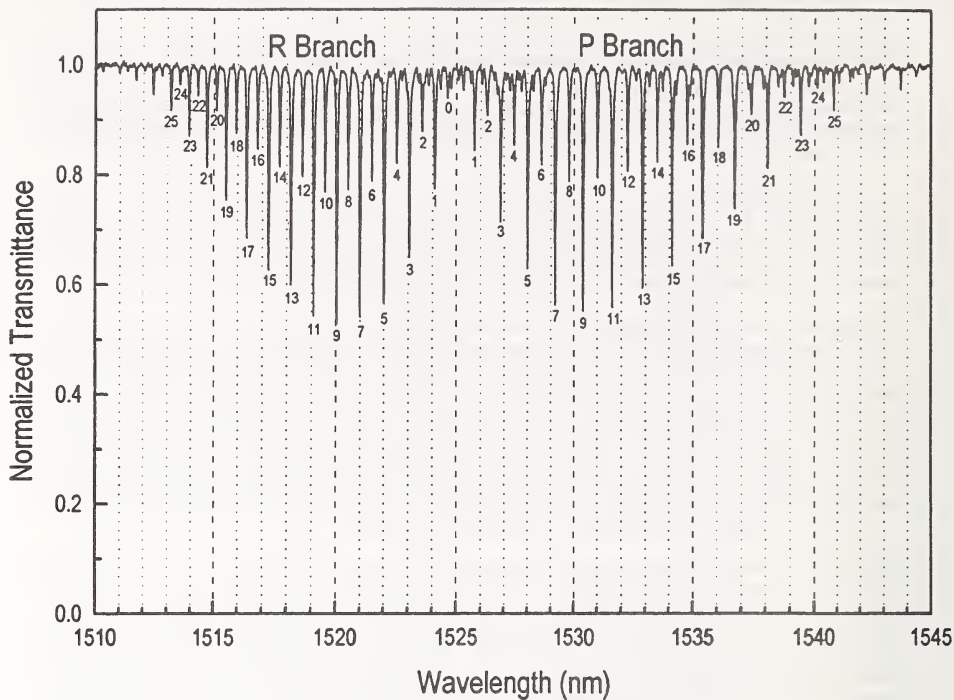


Figure 1. Acetylene ( $^{12}\text{C}_2\text{H}_2$ ) spectrum taken by passing LED light through an absorption cell and recording the spectrum of the transmitted light using an optical spectrum analyzer with 0.05 nm resolution. This spectrum has been divided by the LED spectrum.

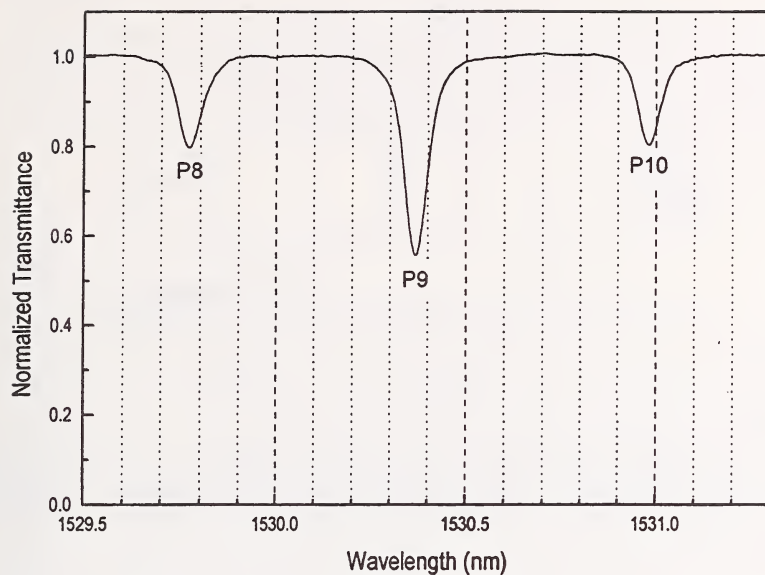
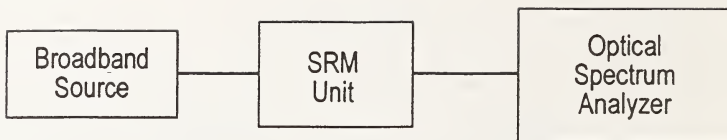
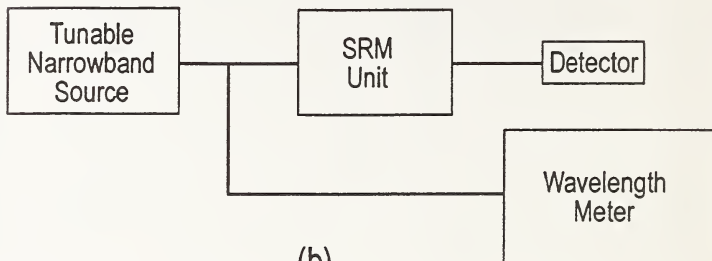


Figure 2. The P8, P9, and P10 lines from Figure 1 on an expanded wavelength scale to show lineshape.



(a)



(b)

Figure 3. (a) Schematic of technique when using the SRM and a broadband source to calibrate an optical spectrum analyzer. (b) Schematic of technique when using the SRM and a narrowband source to calibrate a tunable laser or a wavelength meter. The wavelength meter is not required for a laser calibration.

#### REFERENCES

- [1] Nakagawa, K., Labachellerie, M., Awaji, Y., and Kourogi, M., "Accurate Optical Frequency Atlas of the 1.5- $\mu\text{m}$  Bands of Acetylene," J. Opt. Soc. Am. B 13, pp. 2708-2714, (1996).
- [2] Yoshida, T. and Sasada, H., "Near-Infrared Spectroscopy with a Wavemeter," J. Molec. Spectrosc. 153, pp. 208-210 (1992); Guelachvili, G. and Rao, K.N., Handbook of Infrared Standards II, Academic Press, San Diego, CA, pp. 564-568 (1993).
- [3] Gilbert, S.L., and Swann, W.C., "Standard Reference Materials: Acetylene  $^{12}\text{C}_2\text{H}_2$  Absorption Reference for 1510–1540 nm Wavelength Calibration – SRM 2517," NIST Special Publication 260-133 (1997). In Press.
- [4] Edlen, B., "The Refractive Index of Air," Metrologia, 2, p. 12, (1966); CRC Handbook of Chemistry and Physics 77<sup>th</sup> Ed., pp. 10-266, (1996).

*It is the responsibility of users of this SRM to assure that the certificate in their possession is current. This can be accomplished by contacting the SRM Program at (301) 975-6776 (select "Certificates"), Fax (301) 926-4751, e-mail [srminfo@nist.gov](mailto:srminfo@nist.gov), or via of the Internet <http://ts.nist.gov/srm>.*



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